Claims

1. A novel neolignan 3-ethyl-2-methyl-3-(2", 4", 5"-trimethoxy-phenyl-1-(2',4',5'-trimethoxy) phenyl-1-(2',4',5'-trimethoxy)phenyl-1-propene of formula (II)

(II)

2. A neolignan compound as claimed in claim 1 has following physical characteristics:

R_f: 0.45 (solvent: Ethylacetate-Hexane; 2:8)

m.p; 96° -97° C

¹H NMR (CDCl₃) δ 6.91 (1H, s, H-6'), 6.84 (1H, s, H-6"), 6.55(1H, s, H-3'), 6.51 (1H, s, H-3"), 6.48 (1H, s, H-1), 3.96 (6H, s, 2'-OCH₃ and 2"-OCH₃), 3.84 (6H, s, 4'-OCH₃ and 4"-OCH₃), 3.80(3H, s, 5'-OCH₃), 3.78 (3H, s, 5"-OCH₃), 3.59(1H, t, H-3), 1.70-1.97 (2H, m, H-4), 1.66 (3H, s, H-6), 0.93(3H, t, H-5); ¹H NMR (DMSO-d₆) δ 6.79 (1H, s, H-6'), 6.68 (1H, s, H-6"), 6.67 (1H, s, H-3'), 6.66 (1H, s, H-3"), 6.34 (1H, s, H-1), 3.84 (9H, s, 2"-OCH₃, 4"-OCH₃ and 5"-OCH₃), 3.68 (3H, s, 2'-OCH₃), 3.66 (3H, s, 4'-OCH₃), 3.62 (3H, s, 5'-OCH₃), 3.53 (1H, t, H-3), 1.88-1.67 (2H, m, H-4), 1.60(3H, s, H-6), 0.84 (3H, t, H-5);

¹³CNMR (CDCl₃) δ 152.48 (C-2'), 152.02 (C-2"), 148.48 (C-4'), 147.94 (C-4"), 143.57 (C-5'), 142.89 (C-5"), 140.41 (C-2), 124.88 (C-1'), 120.18 (C-1), 119.65 (C-1"), 114.88 (C-6'), 112.14 (C-6"), 99.47 (C-3"), 99.37 (C-3"), 57.37 (5"-OCH₃), 57.09 (5'-OCH₃), 57.07 (4"-OCH₃), 56.94 (4'-OCH₃), 56.55(2"-OCH₃), 56.48 (2'-OCH₃), 47.38 (C-3), 26.74 (C-4), 17.82 (C-6), 12.84 (C-5);

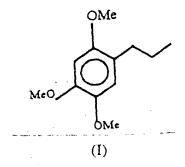
¹³C NMR (DMSO-d₆) δ 152.56 (C-2'), 152.11 (C-2"), 149.07 (C-4'), 148.53 (C-4"), 143.53 (C-5'), 142.84 (C-5"), 139.45(C-2), 123.96 (C-1'), 120.56 (C-1),

119.09 (C-1"), 115.47 (C-6'), 13.02 (C-6"), 99.55 (C-3'), 99.23 (C-3"), 57.39(5"-OCH₃), 57.24 (5'-OCH₃), 57.17 (4"-OCH₃), 57.08 (4'-OCH₃), 56.63 (2"-OCH₃), 56.59 (2'-OCH₃), 47.56 (C-3), 26.46 (C-4), 17.71 (C-6), 13.33 (C-5);

NMR (DEPT-135°) δ 120.56(C-1), 115.47 (C-6'), 113.02 (C-6"), 99.55 (C-3'), 99.23 (C-3"), 57.39 (5"-OCH₃), 57.24 (5'-OCH₃), 57.17 (4"-OCH₃), 57.08 (4'-OCH₃), 57.08 (4'-OCH₃), 56.63 (2"-OCH₃), 56.59 (2'-OCH₃), 47. 56 (C-3, down), 26.46 (C-4), 17.71 (C-6), 13.33 (C-5);

EIMS m/z (%): 416 [M]+ (14), 219 (100), 209 (47), 181 (21), 171 (20), 71 (27).

- 3. A neolignan as claimed in claim 1 is named as NEOLASA –I
- 4. A neolignan as claimed in claim 1 has one asymmetric center.
- 5. A neolignan as claimed in claim 1 has aliphatic side chain with one double bond.
- 6. A neolignan as claimed in claim 1 is capable of undergoing conversion into several naturally occurring neolignan and lignan derivatives.
- 7. A neolignan as claimed in claim 1 is capable of undergoing hydrogenation to yield dihydro neolignan 3-ethyl-2-methyl-3-(2",4", 5"-trimethoxy) phenyl-1-(2', 4', 5'-trimethoxy) phenyl propane (III) to further establish the presence of a reducible double bond.
- 8. A dihydroneolignan as claimed in claim 7 is named as NEOLASA-II.
- 9. A dihydroneolignan as claimed in claim 7 has two asymmetric centers.
- 10. A process for the preparation of nelignan 3-ethyl-2-methyl-3-(2", 4", 5"-trimethoxy) phenyl-1-(2', 4', 5'-trimethoxy) phenyl-1-propene of formual II from toxic β-asarone or β-asarone rich *Acorus calamus* oil containing α and γ-asarone, the said process comprising the following steps:
 - a) hydrogenating β -asarone or β -asarone rich calamus oil containing α and γ -asarone using 10% Pd/c catalyst, with or without ammonium formate under pressure between 0 40 psi at room temperature,
 - b) purifying the product of step (a) over silica gel column to obtain compound of formula (I),



- c) stirring the compound of formula (I) of step (b) with DDQ and an organic acid at room temperature for a period of 16-20 hrs.
- d) filtering the precipitate solid (DDQH₂) and washing the residue with an organic acid,
- e) evaporating combined organic acid solution of step (d), to obtain a concentrated solution,
- f) pouring concentrated solution of step (e) into water,
- g) extracting the aqueous solution of step (f) with aliphatic halogenated hydrocarbon solvent and separating organic layer,
- h) washing the organic layer of step (g) with brine, 10% bicarbonate solution, followed by again brine and drying organic layer over anhydrous sodium sulphate, filtering and evaporating to dryness to obtain a residue, and
- i) purifying residue of step (h) over silica gel column to obtain three sets of fraction which are crystallized separately from a mixture of hexane:methanol to obtain α-asarone (I, 19 %), 1- (2,4,5-trimethoxy) phenyl-1-propanone (IIb, 22%) and neolignan 3-ethyl-2-methyl-3-(2", 4", 5"-trimethoxy) phenyl-1-(2', 4', 5'-trimethoxy) phenyl-1-propene (II, 32%)

(II)

- 11) A process as claimed in claim 10 wherein in step (c) the effective molar ratio of 2,4,5-trimethoxyp propane and DDQ is in the range of 1:1 to 1:2.1
- 12) A process as claimed in claim 10, wherein in steps (c) and (d) the organic acid used is selected form acetic acid or propionic acid and preferably acetic acid.
- 13) A process as claimed in claim 10, wherein in step (g) the aliphatic halogenated hydrocarbon solvent used is selected from dichloromethane, carbontetrachloride or chloroform and preferably dichloromethane.
- 14) A process of claim 10 provides neolignan and other useful side products of high purity.
- 15) A process as claimed in claim 10 wherein in step (I) the neolignan obtained is termed as NEOLASA-I.
- 16) A process as claimed in claim 10, wherein the said neolignan (II) has one asymmetric center.
- 17) A process as claimed in claim 10, wherein the said neolignan (II) neolignan obtained provides the opportunity for evaluation of its biological activity.
- 18) A process as claimed in claim 10, wherein the said neolignan (II) has aliphatic side chain with one double bond.
- 19) A process as claimed in claim 10, wherein the said neolignan (II) is capable of undergoing conversion into several naturally occurring neolignans and lignan derivatives.
- A process as claimed in claim 10, wherein the said neolignan (II) is capable of undergoing hydrogenation to yield dihydroneolignan 3-ethyl-2-methyl-3-(2",4", 5"-trimethoxy)phenyl-1-(2', 4', 5'-trimethyoxy)phenyl propane (III) to further substantiate the presence of a double bond in neolignan (II).

- 21) A dihyroneolignan (III) of claim 17 is named as NEOLASA-II.
- 22) A dihydrolignan (III) of claim 17 has two asymmetric centers